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Benzylammonium 2,4-bis(dicyanomethylene)-2,3-dihydroisoindolide

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The cation and anion of the title salt, $C_7H_{10}N^+.C_{14}H_4N_5^-$, are both bisected by a crystallographic mirror plane. Extensive hydrogen bonding, with the $R_6^6(28)$ graph-set motif, connects the ions into layers.

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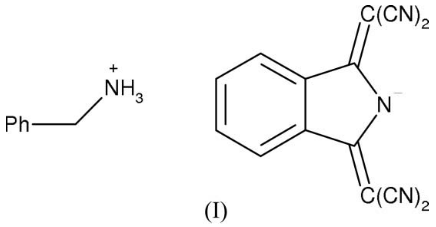
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.005 Å
R factor = 0.051
wR factor = 0.127
Data-to-parameter ratio = 12.4

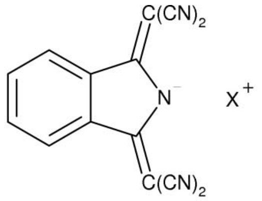
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

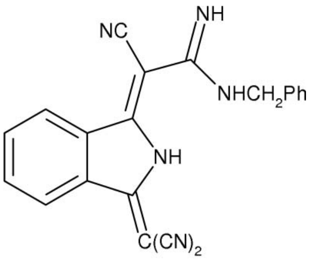
The title compound, (I), is a by-product of the reaction between ammonium salt (II) and benzylamine, producing the amidine, (III), in which the cation of the original salt has been replaced by benzylammonium. The anion and cation of (I), along with indications of the crystallographic symmetry to which they are subject, are shown in Figs. 1 and 2, respectively.



(I)



(I) X = $PhCH_2NH_3$
(II) X = NH_4



(III)

In the anion, the lengths of the N1—C1 and C1—C5 bonds and their symmetry-related equivalents [1.363 (2) and 1.382 (3) Å, respectively] are surprisingly long for their type, which is taken as an indication of their involvement in the delocalization of the negative charge on the anion. Another feature of the structure of the anion is the dihedral angle of 5.77 (15)° between the plane of the five-membered ring and

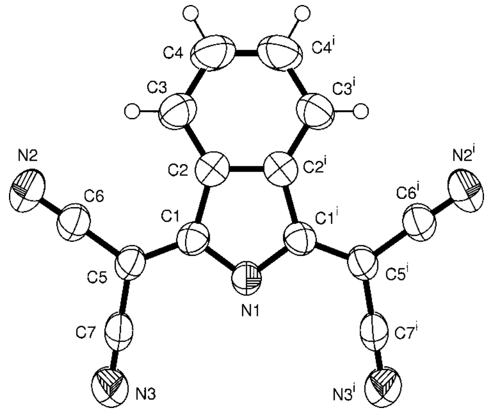


Figure 1
A view of the anion of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small circles of arbitrary radii. [Symmetry code (i) x, $-y$, z.]

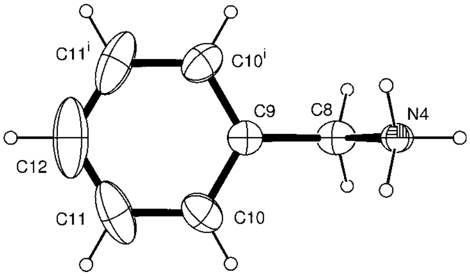


Figure 2
A view of the cation of (I). Displacement ellipsoids are drawn at the 20% probability level and H atoms are shown as small circles of arbitrary radii. [Symmetry code (i) x, $-y$, z.]

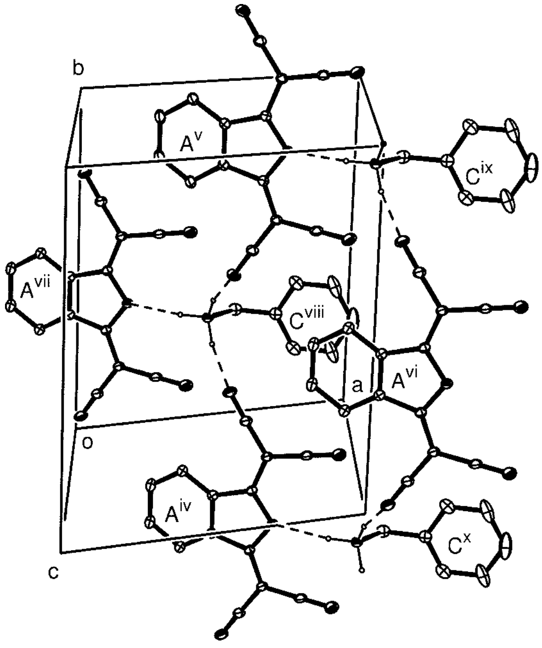


Figure 3
Hydrogen bonding in (I). Displacement ellipsoids are drawn at the 10% probability level. H atoms involved in inter-ion contacts (dashed lines) are shown as small circles of arbitrary radii. Ions are identified according to type as C for cations and A for anions. [Symmetry codes: (iv) $1-x, y, 1-z$; (v) $1-x, 1-y, 1-z$; (vi) $\frac{3}{2}-x, \frac{1}{2}+y, \frac{3}{2}-z$; (vii) $\frac{3}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$; (viii) $\frac{1}{2}+x, \frac{1}{2}+y, \frac{1}{2}+z$; (ix) $1+x, 1+y, 1+z$; (x) $1+x, y, 1+z$.]

that of the $C(CN)_2$ group. In this case, the displacements of the atoms of both $C(CN)_2$ groups are all in the same sense relative to the plane of the five-membered ring. The only notable feature of the structure of the cation is the dihedral angle of 90.00 (11)° between the plane defined by atoms N4/C8/C9 and that of the benzene ring. The most striking feature of the structure of (I) is the inter-ion connectivity created by the N—H···N hydrogen bonds given in Table 1. These hydrogen bonds, which involve all three of the H atoms of the NH_3 group of the benzylammonium cation with three of the five N atoms of the anion as acceptors, create sheets of ions parallel to $(10\overline{1})$, interconnected as shown in Fig. 3. The hydrogen-bond motif, in the graph-set notation of Bernstein *et al.* (1995), which recurs throughout the layer is $R_6^6(28)$ and is exemplified in Fig. 3 by the connectivity of the species $A^{iv}/C^{viii}/A^{v}/C^{ix}/A^{vi}/C^{x}$. The disposition of the H atoms in the NH_3 group demands some degree of depth or thickness within the layers, and this requirement is met in such a way as to accommodate the first of the π–π overlaps given in Table 2 and exemplified in Fig. 3 by the situation for C^{viii} and A^{vi}. The second π–π overlap given in Table 2 occurs between layers and involves rings which are related to one another by a crystallographic twofold axis which, because of the crystallographic symmetry of the ring and the anion of which it is part, can be expressed equally as a crystallographic centre of symmetry. This last is also the relationship between neighbouring layers.

Experimental

Heating a solution of (II) (0.50 g, 1.9 mmol) and benzylamine (0.21 g, 1.9 mmol) in 1,4-dioxan (30 ml) under reflux for 4 h resulted in precipitation of an orange solid which, when filtered off, dried under vacuum and recrystallized from dimethylformamide–ethanol (10:90), yielded *N*-benzyl-2-cyano-2-(3-dicyanomethylene-2,3-dihydroisoindolylidene)acetamidine, (III) [0.31 g, 46%; m.p. 573–574 K (decomposition)]. Evaporation of the filtrate to dryness and recrystallization from acetonitrile gave (I) (0.19 g, 28%; m.p. 571–572 K). ν_{max}: 3134, 3094, 2612, 2209, 1596, 1586, 1504, 1381, 1310, 1248, 1129, 1098, 952, 848, 754 and 708 cm^{-1}; λ_{max} (CH_3CN): 496 (e = 32 597 dm^3 mol^{-1} cm^{-1}), 464 (32 393), 342 (13 124) and 240 nm (28 786); ^{1}H NMR (400 MHz, DMSO-d_6, δ): 8.52 (*br m*, 5H, two benzo H and NH_3), 7.65 (*m*, 2H, benzo H), 7.45 (*m*, 5H, phenyl H) and 4.5 (*s*, 2H, CH_2). On addition of D_2O to the NMR sample, the multiplet at 8.52 p.p.m. was no longer broad and integrated for 2 protons. ^{13}C NMR (100 MHz, DMSO-d_6, δ): 42.28 (CH_2), 53.89 [=**C**(CN)$_2$], 116.24 and 117.19 (CN), 122.83, 128.45, 128.57, 128.76, 131.27, 133.83 and 137.38 (aromatic C) and 171.97 [**C**=C(CN)$_2$]. Analysis found: C 72.15, H 4.12, N 24.52%; $C_{21}H_{14}N_6$ requires: C 71.99, H 4.02, N 23.99%.

Crystal data

$C_7H_{10}N^+\cdot C_{14}H_4N_5^-$
M_r = 350.38
Monoclinic, $I2/m$
a = 11.46 (2) Å
b = 13.094 (5) Å
c = 13.563 (9) Å
β = 114.22 (5)°
V = 1857 (4) Å^3
Z = 4

D_x = 1.254 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 14 reflections
θ = 8.5–12.4°
μ = 0.08 mm^{-1}
T = 295 (2) K
Block, orange
0.44 × 0.44 × 0.30 mm

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Data collection

Nicolet P3 four-circle diffractometer
ω–2θ scans
Absorption correction: none
1803 measured reflections
1714 independent reflections
1044 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.017$

$\theta_{\max} = 25.1°$
$h = 0 \rightarrow 12$
$k = 0 \rightarrow 15$
$l = -16 \rightarrow 14$
2 standard reflections
every 50 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.127$
$S = 0.99$
1714 reflections
138 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0627P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.14$ e Å^{-3}
$\Delta\rho_{\min} = -0.15$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0037 (9)

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4B···N1$^{\rm i}$	0.99 (4)	2.28 (4)	3.227 (6)	159 (3)
N4—H4A···N2$^{\rm ii}$	1.02 (2)	2.02 (2)	3.024 (3)	167.2 (19)

Symmetry codes: (i) $-x, -y, -z$; (ii) $\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z$.

Table 2
Parameters (Å, °) for π–π contacts in (I).

CgI···CgJ	Cg···Cg	α	β	γ	$CgI_{\rm perp}$	$CgJ_{\rm perp}$
$Cg1$···$Cg2$	3.551	6.26	2.54	3.72	3.544	3.548
$Cg1$···$Cg1^{\rm xi}$	3.448	0.00	6.64	6.64	3.424	3.424

Notes: Ring 1, with centroid $Cg1$, is defined by N1/C1/C2/C2$^{\rm i}$/C1$^{\rm i}$; ring 2, with centroid $Cg2$, is defined by C9/C10/C11/C12/C11$^{\rm i}$/C10$^{\rm i}$. $CgX_{\rm perp}$ ($X = I$ or J) is the perpendicular distance of the centroid of ring X to the least squares plane of ring Y ($X \neq Y$). α is the dihedral angle between the planes of the rings. β and γ are the angles at CgX between Cg···Cg and $CgX_{\rm perp}$ for $X = I$ and J, respectively. Symmetry codes: (i) $x, -y, z$; (xi) $1 - x, y, -z$.

In this structure, both ions are bisected by a crystallographic mirror plane. The only atoms in general positions and replicated therefore by crystallographic symmetry to complete the ions are, in the benzylammonium counter-cation, one H atom of each of the NH_3 group and the methylene group and the C atoms, and the H atoms attached to them, *ortho* and *meta* to the methylene group, and in the anion, all atoms except the N atom in the five-membered ring. The somewhat extreme anisotropic displacement parameters associated with atoms C11 and C12 are attributed to a degree of disorder in these sites which has not been modelled in detail. Difference-map peaks provided approximate positions for the H atoms of the NH_3 group. These H atoms were then refined with isotropic displacement parameters in the usual manner. H atoms attached to C atoms were placed in calculated positions, with C—H set at 0.93 and 0.97 Å for aryl and methylene H atoms, respectively, and refined using a riding model, with $U_{\rm iso}(\rm H) = 1.2U_{\rm eq}(\rm C)$ in both cases.

Data collection: *Nicolet P3 software* (Nicolet, 1980); cell refinement: *Nicolet P3 software*; data reduction: *RDNIC* (Howie, 1980); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

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supporting information

Acta Cryst. (2005). E**61**, o2258–o2260   [https://doi.org/10.1107/S1600536805018866]

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Crystal data

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$M_r = 350.38$
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$\beta = 114.22$ (5)°
$V = 1857$ (4) Å^3
$Z = 4$
$F(000) = 728$
$D_x = 1.254$ Mg m^{-3}
Melting point = 571–572 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 14 reflections
$\theta = 8.5$–12.4°
$\mu = 0.08$ mm^{-1}
$T = 295$ K
Block, orange
0.44 × 0.44 × 0.30 mm

Data collection

Nicolet P3 four-circle diffractometer
Radiation source: normal-focus sealed tube
Graphite monochromator
ω–2θ scans
1803 measured reflections
1714 independent reflections
1044 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.017$
$\theta_{\rm max} = 25.1°$, $\theta_{\rm min} = 2.0°$
$h = 0 \rightarrow 12$
$k = 0 \rightarrow 15$
$l = -16 \rightarrow 14$
2 standard reflections every 50 reflections
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.127$
$S = 0.99$
1714 reflections
138 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: geom and difmap
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0627P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.14$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.15$ e Å^{-3}
Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0037 (9)

Special details

Experimental. Scan rates, dependent on prescan intensity (Ip), were in the range 58.6 (Ip>2500) to 5.33 (Ip<150) ° 2θ min^{-1}. Scan widths, dependent on 2θ, were in the range 2.4 to 2.7 ° 2θ. Stationary crystal, stationary counter background counts were taken on either side of the peak each for 25% of the total (peak plus background) count time.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.
Least-squares planes (x,y,z in crystal coordinates) and deviations from them (* indicates atom used to define plane)
8.3940 (175) x - 0.0000 y - 12.4980 (253) z = 2.4776 (57)
* -0.0167 (0.0021) N1 * -0.0098 (0.0014) C1 * 0.0263 (0.0017) C2 * 0.0114 (0.0019) C3 * -0.0195 (0.0014) C4 * -0.0098 (0.0014) C1_$1 * 0.0263 (0.0017) C2_$1 * 0.0114 (0.0019) C3_$1 * -0.0195 (0.0014) C4_$1 - 0.0730 (0.0026) C5 - 0.0998 (0.0025) C6 - 0.1780 (0.0033) C7 - 0.1315 (0.0025) N2 - 0.2715 (0.0039) N3
Rms deviation of fitted atoms = 0.0179
7.8323 (185) x + 0.9875 (249) y - 12.7850 (259) z = 2.3858 (64)
Angle to previous plane (with approximate e.s.d.) = 5.77 (0.15)
* -0.0024 (0.0011) C5 * 0.0024 (0.0019) C6 * 0.0030 (0.0021) C7 * -0.0013 (0.0010) N2 * -0.0016 (0.0012) N3
Rms deviation of fitted atoms = 0.0022
- 7.3079 (209) x + 0.0000 y + 13.0768 (269) z = 1.5705 (71)
Angle to previous plane (with approximate e.s.d.) = 5.65 (0.19)
* 0.0008 (0.0028) C9 * -0.0006 (0.0020) C10 * 0.0002 (0.0036) C11 * 0.0000 (0.0051) C12 * -0.0006 (0.0020) C10_$1 * 0.0002 (0.0036) C11_$1 - 0.0402 (0.0061) C8 1.3100 (0.0071) N4
Rms deviation of fitted atoms = 0.0005
- 0.0000 x - 13.0940 (0.0263) y + 0.0000 z = 0.0000
Angle to previous plane (with approximate e.s.d.) = 90.00 (0.11)
* 0.0000 (0.0000) N4 * 0.0000 (0.0000) C8 * 0.0000 (0.0000) C9
Rms deviation of fitted atoms = 0.0000

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	$U_{\rm iso}$*/$U_{\rm eq}$
N1	0.3135 (2)	0.0000	0.01368 (18)	0.0496 (6)
C1	0.38537 (18)	0.08350 (15)	0.06137 (15)	0.0477 (5)
C2	0.51242 (18)	0.05337 (15)	0.14381 (15)	0.0501 (5)
C3	0.61578 (19)	0.10769 (18)	0.21442 (18)	0.0650 (7)
H3	0.6164	0.1787	0.2140	0.078*
C4	0.7191 (2)	0.05223 (18)	0.2863 (2)	0.0789 (8)
H4	0.7899	0.0869	0.3355	0.095*
C5	0.3396 (2)	0.18195 (15)	0.03565 (15)	0.0526 (6)
C6	0.4119 (2)	0.26993 (17)	0.08642 (17)	0.0596 (6)
N2	0.46788 (19)	0.34170 (16)	0.12652 (17)	0.0799 (7)
C7	0.2127 (2)	0.19929 (15)	−0.04116 (19)	0.0686 (7)
N3	0.1099 (2)	0.21293 (16)	−0.10270 (19)	0.1049 (9)
N4	−0.0440 (3)	0.0000	0.1957 (2)	0.0577 (7)
H4A	−0.029 (2)	0.0599 (18)	0.2475 (19)	0.095 (8)*
H4B	−0.136 (4)	0.0000	0.145 (3)	0.098 (12)*
C8	0.0479 (3)	0.0000	0.1438 (3)	0.0762 (10)
H8A	0.0324	−0.0598	0.0980	0.091*
C9	0.1838 (3)	0.0000	0.2229 (3)	0.0660 (9)
C10	0.2474 (3)	0.0901 (2)	0.2583 (2)	0.0958 (9)
H10	0.2051	0.1519	0.2345	0.115*

C11	0.3733 (3)	0.0892 (5)	0.3287 (3)	0.149 (2)
H11	0.4159	0.1509	0.3526	0.178*
C12	0.4380 (6)	0.0000	0.3649 (5)	0.179 (5)
H12	0.5238	0.0000	0.4128	0.215*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0581 (15)	0.0383 (13)	0.0447 (13)	0.000	0.0134 (12)	0.000
C1	0.0536 (12)	0.0471 (12)	0.0411 (10)	−0.0031 (10)	0.0183 (10)	−0.0022 (9)
C2	0.0530 (12)	0.0517 (11)	0.0488 (11)	−0.0041 (10)	0.0240 (10)	−0.0026 (10)
C3	0.0530 (13)	0.0630 (15)	0.0745 (15)	−0.0074 (12)	0.0217 (12)	−0.0093 (12)
C4	0.0490 (13)	0.0902 (17)	0.0863 (17)	−0.0091 (12)	0.0163 (12)	−0.0108 (14)
C5	0.0616 (13)	0.0410 (11)	0.0477 (12)	−0.0038 (11)	0.0147 (10)	−0.0055 (9)
C6	0.0682 (15)	0.0484 (13)	0.0575 (14)	−0.0029 (12)	0.0212 (12)	−0.0057 (11)
N2	0.0891 (15)	0.0549 (12)	0.0850 (14)	−0.0152 (12)	0.0247 (12)	−0.0154 (11)
C7	0.0811 (17)	0.0351 (12)	0.0680 (15)	0.0014 (12)	0.0088 (14)	−0.0057 (11)
N3	0.0987 (17)	0.0586 (14)	0.1009 (17)	0.0108 (12)	−0.0162 (15)	−0.0012 (12)
N4	0.0606 (18)	0.0480 (16)	0.0532 (16)	0.000	0.0119 (15)	0.000
C8	0.097 (3)	0.072 (2)	0.057 (2)	0.000	0.029 (2)	0.000
C9	0.075 (2)	0.072 (2)	0.060 (2)	0.000	0.0366 (19)	0.000
C10	0.101 (2)	0.095 (2)	0.104 (2)	−0.0255 (19)	0.0543 (18)	−0.0144 (18)
C11	0.092 (3)	0.242 (6)	0.128 (4)	−0.075 (3)	0.062 (3)	−0.058 (4)
C12	0.069 (4)	0.393 (16)	0.081 (4)	0.000	0.038 (3)	0.000

Geometric parameters (Å, º)

N1—C1	1.362 (2)	N4—H4A$^{\rm i}$	1.02 (2)
N1—C1$^{\rm i}$	1.362 (2)	N4—C8	1.488 (5)
C1—C5	1.382 (3)	N4—H4A	1.02 (2)
C1—C2	1.480 (3)	N4—H4B	0.99 (4)
C2—C3	1.377 (3)	C8—C9	1.486 (5)
C2—C2$^{\rm i}$	1.398 (4)	C8—H8A	0.9700
C3—C4	1.391 (3)	C9—C10	1.367 (3)
C3—H3	0.9300	C9—C10$^{\rm i}$	1.367 (3)
C4—C4$^{\rm i}$	1.368 (5)	C10—C11	1.365 (5)
C4—H4	0.9300	C10—H10	0.9300
C5—C7	1.417 (4)	C11—C12	1.363 (5)
C5—C6	1.422 (3)	C11—H11	0.9300
C6—N2	1.142 (3)	C12—C11$^{\rm i}$	1.363 (5)
C7—N3	1.144 (3)	C12—H12	0.9300

C1—N1—C1$^{\rm i}$	106.8 (2)	H4A$^{\rm i}$—N4—H4B	108.1 (18)
N1—C1—C5	122.41 (19)	C8—N4—H4B	115 (2)
N1—C1—C2	111.14 (18)	H4A—N4—H4B	108.1 (18)
C5—C1—C2	126.42 (17)	C9—C8—N4	113.2 (3)
C3—C2—C2$^{\rm i}$	121.10 (13)	C9—C8—H8A	108.9
C3—C2—C1	133.39 (19)	N4—C8—H8A	108.9

C2^{i}—C2—C1	105.46 (11)	C9—C8—H8A^{i}	108.9
C2—C3—C4	117.4 (2)	N4—C8—H8A^{i}	108.9
C2—C3—H3	121.3	H8A—C8—H8A^{i}	107.7
C4—C3—H3	121.3	C10—C9—C10^{i}	119.4 (4)
C4^{i}—C4—C3	121.48 (14)	C10—C9—C8	120.3 (2)
C4^{i}—C4—H4	119.3	C10^{i}—C9—C8	120.3 (2)
C3—C4—H4	119.3	C11—C10—C9	119.8 (4)
C1—C5—C7	120.28 (18)	C11—C10—H10	120.1
C1—C5—C6	123.22 (19)	C9—C10—H10	120.1
C7—C5—C6	116.44 (19)	C12—C11—C10	121.5 (6)
N2—C6—C5	178.6 (2)	C12—C11—H11	119.3
N3—C7—C5	179.5 (3)	C10—C11—H11	119.3
H4A^{i}—N4—C8	111.7 (13)	C11^{i}—C12—C11	118.0 (7)
H4A^{i}—N4—H4A	101 (3)	C11^{i}—C12—H12	121.0
C8—N4—H4A	111.7 (13)	C11—C12—H12	121.0

N1—C1—C5—C6	178.4 (2)	C2—C1—C5—C7	−176.41 (19)
N1—C1—C5—C7	1.4 (3)	N4—C8—C9—C10	−91.0 (3)
C2—C1—C5—C6	0.6 (3)		

Symmetry code: (i) *x*, −*y*, *z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4*B*···N1^{ii}	0.99 (4)	2.28 (4)	3.227 (6)	159 (3)
N4—H4*A*···N2^{iii}	1.02 (2)	2.02 (2)	3.024 (3)	167.2 (19)

Symmetry codes: (ii) −*x*, −*y*, −*z*; (iii) −*x*+1/2, −*y*+1/2, −*z*+1/2.